ABSTRACT

A molecular simulation method for dividing a molecule or a part of molecule to be simulated into a QM space and an MM apace and applying an *ab initio* molecular orbital method to the QM space and a method based on an empirical potential to the MM space to perform molecular simulation includes the steps of: retrieving structure data on the molecule or part of molecule to be simulated from a storage unit, and dividing the structure data into the QM space and the MM space; and replacing a part of a total energy expression in the *ab initio* molecular orbital method concerning the QM space with an empirical potential.